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Equivalence of Bose-Einstein condensation and symmetry breaking

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Based on a classic paper by Ginibre [Commun. Math. Phys. **8** 26 (1968)] it is shown that whenever Bogoliubov's approximation, that is, the replacement of a_0 and a_0^* by complex numbers in the Hamiltonian, asymptotically yields the right pressure, it also implies the asymptotic equality of $|\langle a_0\rangle|^2/V$ and $\langle a_0^* a_0\rangle/V$ in symmetry breaking fields, irrespective of the existence or absence of Bose-Einstein condensation. Because the former was proved by Ginibre to hold for absolutely integrable superstable pair interactions, the latter is equally valid in this case. Apart from Ginibre's work, our proof uses only a simple convexity inequality due to Griffiths.

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The equivalence of Bose-Einstein condensation (BEC) and a spontaneous breakdown of the gauge symmetry related to the choice of a global phase factor in creation and annihilation operators is an intriguing problem which apparently has not yet been solved rigorously. Most of the time the equivalence is tacitly assumed; for example, Hohenberg's celebrated result [1] about one- and two-dimensional Bose-systems is often considered as the proof of the absence of BEC in low dimensions although it proves the absence of symmetry breaking. The equivalence of BEC and symmetry breaking can be summarized as the asymptotic equality of $|\langle a_0\rangle|^2/V$ and $\langle a_0^* a_0\rangle/V$ in the limit of infinite volume, when the thermal or ground state averages are taken in the presence of a symmetry breaking field. The operator a_0^* creates a boson in a one-particle state distinguished by the fact that its occupation may become macroscopic. The problem is that in finite volumes the first quantity is always less than the second; if equality installs asymptotically, it is the work of a large deviation principle resulting in the equivalence of certain statistical ensembles. This question, closely related to the validity of the Bogoliubov approximation (BA) [2], raised only a limited interest almost exclusively among mathematical physicists [3]-[8]. The equivalence of the two notions in the above sense was recently shown by the present author for some models with a simplified interaction [9], without using BA. In that paper it was overlooked that the equivalence for a general interacting Bose gas was a more or less direct consequence of a powerful result about BA by Ginibre, obtained almost forty years ago [3]. One may say that Ginibre himself overlooked this important implication of his work. This note is to present the necessary argument.

In his classic but not widely known paper Ginibre considered a Bose gas with a rather general pair interaction making nearly the minimum assumption to guarantee a non-pathological thermodynamic behaviour. The pair interaction ϕ is superstable and weakly tempered, i.e. for n particles in a box of volume V the total potential energy

$$U(\mathbf{r}_1,\ldots,\mathbf{r}_n)=\sum_{i<j}\phi(\mathbf{r}_i-\mathbf{r}_j)\geq -bn+an^2/V \qquad (1)$$

for any set of position vectors in the box, and

$$\phi(\mathbf{r})\leq \phi_0 r^{-(d+\epsilon)} \qquad (2)$$

for $|\mathbf{r}|=r\geq R$. Here $a>0$ and b are independent of the volume, d is the space dimension and ϕ_0, ϵ and R are positive constants. Ginibre was interested in proving the correctness of BA which consists in treating a_0 and a_0^* as complex numbers. Here a_0^* creates a boson in the one-particle state $\varphi_0\equiv 1/\sqrt{V}$ (but φ_0 could be any other one-particle state). Ginibre's interpretation of BA is as follows. Let F_0 be the single-mode Fock space spanned by the product states $\varphi_0^{\otimes n}$, $n=0,1,2,\ldots$ and let F' be the Fock space built on the orthogonal complement of φ_0 in the one-particle Hilbert space [13]. Let, moreover, $P_{F'}$ be the orthogonal projection onto F'. Then, for an operator B on F and a complex number C the Bogoliubov approximation of B is

$$B_0(C)=P_{F'}A_C B A_C^* P_{F'} \qquad (3)$$

where it is understood that $B_0(C)$ acts only on elements of F'. The operator

$$A_C^*=e^{Ca_0^*-\overline{C}a_0}=e^{-|C|^2/2}e^{Ca_0^*}e^{-\overline{C}a_0} \qquad (4)$$

applied to a ψ in F' creates the coherent state

$$|C\rangle=e^{-|C|^2/2}\sum_{n\geq 0}\frac{C^n}{\sqrt{n!}}\varphi_0^{\otimes n}\ , \qquad (5)$$

tensor-multiplying ψ. If ψ_1, ψ_2 are in F',

$$\langle\psi_1|B_0(C)|\psi_2\rangle = \langle\psi_1 \otimes C|B|\psi_2 \otimes C\rangle. \tag{6}$$

In the first part of his paper Ginibre applied the transformation (3) onto the density matrix $W = e^{-\beta H}$. The Hamiltonian of the system is

$$H = T + U - \mu N - \nu\sqrt{V}(a_0 + a_0^*) \tag{7}$$

where T is the kinetic energy, μ is real, N is the particle number operator and the amplitude ν of the gauge symmetry breaking field is chosen to be real. Because A_C^* is unitary, without the projection the transformation preserves norm, trace and positivity. Together with the projection the trace of a positive operator cannot but decrease. So

$$\mathrm{Tr}\, W_0(C) = \mathrm{Tr}\,' A_C W A_C^* \leq \mathrm{Tr}\, W = Z \tag{8}$$

where $\mathrm{Tr}\,'$ is the trace in F' and thus

$$V^{-1} \log \mathrm{Tr}\, W_0(C) \leq V^{-1} \log Z \equiv \beta p_V(\mu, \nu) \ . \tag{9}$$

Ginibre proved that the limit of the pressure p_V exists and

$$\lim_{V\to\infty} \sup_C\, (\beta V)^{-1} \log \mathrm{Tr}\, W_0(C) = \lim_{V\to\infty} p_V \equiv p(\mu, \nu) \tag{10}$$

showing thereby that with the right choice of C, BA for the density matrix reproduces the exact pressure in the thermodynamic limit.

Bogoliubov's original idea was to make the replacement in the Hamiltonian. Because $a_0|C\rangle = C|C\rangle$, writing H as a normal-ordered polynomial of creation and annihilation operators and applying (3), the resulting $H_0(C)$ is indeed the same as the outcome of a simple substitution. In coherent states particles can enter in contact with each other. While (10) holds also for hard-core interactions, to make $H_0(C)$ meaningful, hard cores have to be excluded. With the additional condition of the absolute integrability of ϕ, Ginibre proved the analog of Eq. (10). The inequalities

$$Z_0(C) = \mathrm{Tr}\,' e^{-\beta H_0(C)} \leq \mathrm{Tr}\, W_0(C) \leq Z \tag{11}$$

or

$$p_0(C) = (\beta V)^{-1} \log Z_0(C) \leq p_V \ , \tag{12}$$

derived in [3], suggest that, again, $p_0(C)$ is to be maximized. The main result (Theorem 3) of [3] is

$$\lim_{V\to\infty} \sup_C\, p_0(C, \mu, \nu) = \lim_{V\to\infty} p_V(\mu, \nu) = p(\mu, \nu) \tag{13}$$

which is our point of departure.

The proof of the equivalence of BEC and symmetry breaking in the sense discussed in the introduction is as follows.

(i) When a sequence of convex functions f_n converges (necessarily to a convex function f), the sequence f_n' of derivatives also converges apart from possibly a set a zero measure. In particular, the inequalities

$$f'(x-0) \leq \liminf_{n\to\infty} f_n'(x-0) \leq \limsup_{n\to\infty} f_n'(x+0) \leq f'(x+0) \tag{14}$$

due to Griffiths [10] hold true. There is at most a countable infinite set of x such that $f'(x-0) < f'(x+0)$; otherwise we have equalities in (14). In the first two applications below the subscript n will correspond to V.

(ii) We embed H into a one-parameter family of auxiliary Hamiltonians

$$H' = T + U - \mu N' - \mu_0 N_0 - \nu\sqrt{V}(a_0 + a_0^*) \tag{15}$$

where $N_0 = a_0^* a_0$ and $N' = N - N_0$. It is easily checked that the pressure $p_V'(\mu, \mu_0, \nu)$ corresponding to H' has all the nice properties shown in [3] for $p_V(\mu, \nu)$. Especially, for fixed μ and ν, p_V' is a convex increasing and real analytic function of μ_0 (so it is continuous, $p_V'(\mu, \mu, \nu) = p_V(\mu, \nu)$), and for fixed μ and μ_0 it is a convex even and real analytic function of ν. These properties, apart from the analyticity but including continuity, are inherited by the (existing) thermodynamic limit $p'(\mu, \mu_0, \nu)$, so $p'(\mu, \mu, \nu) = p(\mu, \nu)$. Also,

$$\frac{\langle a_0\rangle_{\mu,\mu_0,\nu}}{\sqrt{V}} = \frac{\langle a_0^*\rangle_{\mu,\mu_0,\nu}}{\sqrt{V}} = \frac{1}{2}\frac{\partial p_V'(\mu, \mu_0, \nu)}{\partial \nu} \tag{16}$$

and

$$\frac{\langle N_0\rangle_{\mu,\mu_0,\nu}}{V} = \frac{\partial p_V'(\mu, \mu_0, \nu)}{\partial \mu_0} \tag{17}$$

where the averages are taken with the density matrix $e^{-\beta H'} / \mathrm{Tr}\, e^{-\beta H'}$. For any fixed μ and for $(\mu_0, \nu \neq 0)$ in a set Ω_μ of full Lebesgue measure both $\partial p'/\partial\nu$ and $\partial p'/\partial\mu_0$ exist, and by Eq. (14)

$$\lim_{V\to\infty} \langle a_0\rangle_{\mu,\mu_0,\nu}/\sqrt{V} = (1/2)\partial p'(\mu, \mu_0, \nu)/\partial\nu \tag{18}$$

and

$$\lim_{V\to\infty} \langle N_0\rangle_{\mu,\mu_0,\nu}/V = \partial p'(\mu, \mu_0, \nu)/\partial\mu_0 \ . \tag{19}$$

With the possible exception of a countable number of values of ν Eq. (18) holds also for $\mu_0 = \mu$. This may not be true for Eq. (19): there is an abstract possibility that for a positive-measure set of ν the μ_0-derivative of p' does not exist at $\mu_0 = \mu$. This, however, would have no practical importance because for *any* choice of (μ, ν), $\partial p'/\partial\mu_0$ exists for almost every μ_0 and, hence, for μ_0 arbitrarily close to μ. We return to this point later.

(iii) Apply BA to H' to obtain $H_0'(C)$, $Z_0'(C)$ and $p_0'(C)$. Theorem 3 of [3] extends without any further ado to this case, resulting $p_0'(C) \leq p_V'$ and

$$\lim_{V\to\infty} \sup_C\, p_0'(C) = p' \tag{20}$$

for all μ, μ_0 and ν. With the choice $\nu \neq 0$ real the maximum is attained for C real, $C\nu \geq 0$. Within this set $\mathcal{C}$, p_0' reads

$$p_0'(C,\mu,\mu_0,\nu) = p_0'(C,\mu,0,0) + \mu_0 \frac{C^2}{V} + 2|\nu| \frac{|C|}{\sqrt{V}} \; . \quad (21)$$

For fixed C and μ this is a convex function of both μ_0 and ν;

$$\sup_C p_0'(C) = p_0'(C_{\max}(\mu,\mu_0,\nu),\mu,\mu_0,\nu) \quad (22)$$

is the upper envelope of $\{p_0'(C,\mu,\mu_0,\nu)|C \in \mathcal{C}\}$ and is, therefore, convex in μ_0 and ν. The finite-volume pressure $p_0'(C,\mu,0,0) = p_0'(-C,\mu,0,0)$ is a real analytic function of C. So $p_0'(C,\mu,0,0) \approx p_0'(0,\mu,0,0) + aC^2$ close to $C = 0$. Thus, if $\nu \neq 0$, $C_{\max} \neq 0$ either, and $\partial p_0'/\partial C = 0$ at $C = C_{\max}$. This implies

$$\frac{\partial p_0'(C_{\max}(\mu,\mu_0,\nu),\mu,\mu_0,\nu)}{\partial \nu} = 2\,\mathrm{sgn}\,\nu \frac{|C_{\max}|}{\sqrt{V}} \quad (23)$$

and

$$\frac{\partial p_0'(C_{\max}(\mu,\mu_0,\nu),\mu,\mu_0,\nu)}{\partial \mu_0} = \frac{C_{\max}^2}{V} \; . \quad (24)$$

Now we use (14) a second time, with $f_n = p_0'(C_{\max},\mu,\mu_0,\nu)$ and $f = p'(\mu,\mu_0,\nu)$. For any μ and any $(\mu_0,\nu) \in \Omega_\mu$

$$c_{\max}'(\mu,\mu_0,\nu) = \lim_{V\to\infty} |C_{\max}(\mu,\mu_0,\nu)|/\sqrt{V} \quad (25)$$

exists, and

$$\lim_{V\to\infty} \frac{\langle a_0\rangle_{\mu,\mu_0,\nu}}{\sqrt{V}} = \mathrm{sgn}\,\nu\, c_{\max}' = \mathrm{sgn}\,\nu \lim_{V\to\infty} \sqrt{\frac{\langle N_0\rangle_{\mu,\mu_0,\nu}}{V}} \; . \quad (26)$$

(iv) The above result can be improved. When $\partial p(\mu,\nu)/\partial\nu$ exists, we can set $\mu_0 = \mu$ in Eqs. (18), (23) and (25) and obtain the first half of Eq. (26),

$$\frac{1}{2}\frac{\partial p(\mu,\nu)}{\partial \nu} = \lim_{V\to\infty} \frac{\langle a_0\rangle_{\mu,\nu}}{\sqrt{V}} = \mathrm{sgn}\,\nu\, c_{\max}(\mu,\nu) \; . \quad (27)$$

Here $c_{\max}(\mu,\nu) = c_{\max}'(\mu,\mu,\nu)$ which is clear from $p_0(C,\mu,\nu) = p_0'(C,\mu,\mu,\nu)$. Now fixing any μ, for all ν outside a possible (μ-dependent) set of zero measure there exist both the derivative $\partial p(\mu,\nu)/\partial\nu$ and a sequence $\mu_n \downarrow \mu$ such that $(\mu_n,\nu) \in \Omega_\mu$. For such a ν and μ_n, $p'(\mu,\mu_n,\nu) \to p(\mu,\nu)$ by continuity and $\partial p'(\mu,\mu_n,\nu)/\partial\nu \to \partial p(\mu,\nu)/\partial\nu$ by Griffiths' Lemma (14). Combining Eqs. (18), (26) and (27) one obtains that for almost all $(\mu,\nu\neq 0)$

$$\lim_{V\to\infty} \frac{\langle a_0\rangle_{\mu,\nu}}{\sqrt{V}} = \mathrm{sgn}\,\nu\, c_{\max}(\mu,\nu)$$
$$= \mathrm{sgn}\,\nu \lim_{n\to\infty}\lim_{V\to\infty} \sqrt{\frac{\langle N_0\rangle_{\mu,\mu_n,\nu}}{V}} \; . \quad (28)$$

Equation (28) is nearly the final result except that in the right member the two limits should be interchangeable. This, however, is easily seen. Because of the Schwarz inequality,

$$\lim_{V\to\infty} \frac{|\langle a_0\rangle_{\mu,\nu}|}{\sqrt{V}} \leq \lim_{V\to\infty} \sqrt{\frac{\langle N_0\rangle_{\mu,\nu}}{V}} \; . \quad (29)$$

Suppose that there is a strict inequality here. Note that $\langle N_0\rangle_{\mu,\mu_0,\nu}$ is an increasing function of μ_0. Then for some $\delta > 0$ and for all $V > V_\delta$ and all $\mu_0 \geq \mu$

$$\frac{|\langle a_0\rangle_{\mu,\nu}|}{\sqrt{V}} + \delta < \sqrt{\frac{\langle N_0\rangle_{\mu,\nu}}{V}} \leq \sqrt{\frac{\langle N_0\rangle_{\mu,\mu_0,\nu}}{V}} \; . \quad (30)$$

The contradiction is obvious because $\mu_n \downarrow \mu$ in Eq. (28). Our final result is, thus, that for almost all $(\mu,\nu\neq 0)$

$$\lim_{V\to\infty} \frac{\langle a_0\rangle_{\mu,\nu}}{\sqrt{V}} = \mathrm{sgn}\,\nu\, c_{\max}(\mu,\nu) = \mathrm{sgn}\,\nu \lim_{V\to\infty} \sqrt{\frac{\langle N_0\rangle_{\mu,\nu}}{V}} \; . \quad (31)$$

Equation (31) proves that an optimized c-number substitution provides the right answer at least for the asymptotic value of $\langle a_0\rangle/\sqrt{V}$ and $\langle a_0^* a_0\rangle/V$. It does not tell anything about these values (although for $\nu \neq 0$ they are surely of order 1, as in [9]), especially, about their limit when ν tends to zero. So the equation does not prove that there is a spontaneous symmetry breaking, but it does prove that symmetry breaking occurs simultaneously with Bose-Einstein condensation.

In approximate calculations one often starts with the canonical transformation $a_0 = b_0 + \langle a_0\rangle$ where, by definition, the operator b_0 has zero mean; see e.g. [11]. The approximations made afterwards are based on the hypothesis that the fluctuations of b_0 are negligible or small compared with $\langle a_0^* a_0\rangle$. Equation (31) justifies this hypothesis by proving $\langle b_0^* b_0\rangle_{\mu,\nu}/V \to 0$ as $V \to \infty$.

The functional form of p' is

$$p'(\mu,\mu_0,\nu) = g(c_{\max}(\mu,\mu_0,\nu),\mu)$$
$$+\mu_0 c_{\max}^2(\mu,\mu_0,\nu) + 2|\nu| c_{\max}(\mu,\mu_0,\nu) \; . \quad (32)$$

Alternately, p' has to satisfy the equation

$$\frac{\partial p'(\mu,\mu_0,\nu)}{\partial \mu_0} = \frac{1}{4}\left(\frac{\partial p'(\mu,\mu_0,\nu)}{\partial\nu}\right)^2 \quad (33)$$

obtained by reading the two ends of Eq. (26). Apart from the fact that $\partial p'/\partial\nu$ tends to $\partial p/\partial\nu$, as μ_0 tends to μ, the Bose gas described by the extended Hamiltonian H' may have its own interest. In any case, if μ_0 is close to μ, the behaviour of this system is not expected to significantly differ from that of the original one. BEC or a spontaneous symmetry breaking is described by solutions of (33) that are convex in all the three variables and have a discontinuous ν-derivative at $\nu = 0$.

A different solution to the problem treated in this Letter can be found in Ref. [12].

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[13] This is a corrected definition of F', that agrees with Ginibre's original definition. The correction is to be done also in the PRL.